3-Ethyl-3-heptanol

Other names: 3-Heptanol, 3-ethyl-
3-ethylheptan-3-ol
Inchi: InChI=1S/C9H20O/c1-4-7-8-9(10,5-2)6-3/h10H,4-8H2,1-3H3
InchiKey: XKRZDNKKANUBPV-UHFFFAOYSA-N
Formula: C9H20O
SMILES: CCCCC(O)(CC)CC
Mol. weight [g/mol]: 144.25
CAS: 19780-41-7

Physical Properties

Property code	Value	Unit	Source
gf	-109.08	kJ/mol	Joback Method
hf	-390.07	kJ/mol	Joback Method
hfus	15.74	kJ/mol	Joback Method
hvap	51.01	kJ/mol	Joback Method
log10ws	-2.97		Crippen Method
logp	2.728		Crippen Method
mcvol	143.540	ml/mol	McGowan Method
pc	2574.11	kPa	Joback Method
rinpol	853.00		NIST Webbook
rinpol	853.00		NIST Webbook
tb	494.27	K	Joback Method
tc	662.00	K	Joback Method
tf	254.43	K	Joback Method
vc	0.547	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	337.27	J/mol×K	494.27	Joback Method
cpg	398.12	J/mol×K	634.04	Joback Method
cpg	387.08	J/mol×K	606.09	Joback Method
cpg	375.49	J/mol×K	578.13	Joback Method
cpg	363.35	J/mol×K	550.18	Joback Method

cpg	350.61	J/mol×K	522.22	Joback Method
cpg	408.65	J/mol×K	662.00	Joback Method
dvisc	0.0001471	Pa×s	494.27	Joback Method
dvisc	0.0002563	Pa×s	454.30	Joback Method
dvisc	0.0004970	Pa×s	414.32	Joback Method
dvisc	0.0011101	Pa×s	374.35	Joback Method
dvisc	0.0030048	Pa×s	334.38	Joback Method
dvisc	0.0106579	Pa×s	294.40	Joback Method
dvisc	0.0562745	Pa×s	254.43	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53171e+01
Coeff. B	-4.26150e+03
Coeff. C	-6.77370e+01
Temperature range (K), min.	351.28
Temperature range (K), max.	493.65

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C19780417&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

gf: Standard Gibbs free energy of formation

hf: Enthalpy of formation at standard conditions

hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume